"Dilute" excitons in a double layer system: single-exciton and mean-field approach

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Double layer systems where one layer has electrons and the holes are in a parallel layer a distance d away are expected to undergo excitonic condensation at low temperature. This excitonic condensate is traditionally described by a many-body wavefunction that encodes the coherence between electron and hole bands. Here we compare the mean-field ground state in the limit of dilute electron (hole) density with the ground state of a single electron-hole pair in double-layer system. As the interlayer distance d increases, we find that the excitonic size, characterized by the width of the momentum-space wavefunction, also increases. By comparing the single-exciton wavefunction with the mean-field analysis, we determine the d-dependence of the "diluteness" of the exciton gas in a balanced double-layer system with given electron (or hole) density.

I. INTRODUCTION

The Bose-Einstein condensation of excitons in double layer systems realized in semiconductor heterojunctions, where a macroscopic number of excitons occupy a single quantum state, has been a subject of intense research over the past decade.[1,2] An exciton is a metastable bound state of an electron and a hole. In a balanced electron-hole system at low electron (hole) densities $n_e = n_h = n_{2D}$, the distance between the excitons is much larger than the quantum exciton size and the excitons behave as weakly-interacting bosons.[2,3,4] In a bulk semiconductor or a two-dimensional system, the internal state of the exciton is given by Hydrogenic wavefunctions[2] that result from the Coulomb interaction $V_A(\mathbf{r}) = e^2/\epsilon r$. In each case, the wavefunction for the electron-hole separation decays exponentially with decay length $a_{ex}/2$ where $a_{ex} = \epsilon\hbar^2/e^2 m_r$ is the quantum size of the exciton. Here $\epsilon \sim 10$ is the dielectric constant of the semiconductor heterojunction, $\mathbf{r}_e$ ($\mathbf{r}_h$) represents the electron (hole) position, $m_r^{-1} = m_e^{-1} + m_h^{-1}$ is the (reduced) mass of exciton, and m_e (m_h) is the electron (hole) band mass. Note that for a symmetric electron-hole system that we consider in this paper, $m_e = m_h = 2m_r$, the quantum size of carriers is half the exciton size, $a_0 = \epsilon\hbar^2/e^2 m_e = a_{ex}/2$. Therefore the dimensionless distance between excitons for a given carrier density n_{2D} is given by $r_s/2$ where r_s, defined by $\pi(r_s a_0)^2 = 1/n_{2D}$ is the dimensionless distance between the carriers. Since the quantum size a_{ex} of the exciton is fixed by the semiconductor properties, it is possible to tune the interaction between excitons from weak ($r_s \gg 1$) to strong ($r_s \sim 1$).[4] Note that for a bulk or planar system, as opposed to a double-layer system, the inter-exciton interaction and the formation of exciton are both governed by the same Coulomb interaction $V_A(\mathbf{r})$.

In double-layer systems where electrons are carriers in the top layer and holes are the carriers in the bottom layer, the formation of an exciton is determined by the attractive interlayer Coulomb interaction $V_E(\mathbf{r}) = -e^2/\epsilon\sqrt{r^2+d^2}$ where d is the distance between the two layers and $\mathbf{r}$ denotes the two-dimensional position vector. Since the attractive interaction is d dependent, the quantum size of exciton is not necessarily a_{ex} and, in fact, depends on the dimensionless ratio d/a_0. The interaction between the excitons, on the other hand, is also dependent on intralayer Coulomb repulsion $V_A(\mathbf{r})$. Thus, in double-layer systems, the diluteness of excitons is a function of $(d/a_0, r_s)$. In this paper, we quantitatively explore this issue. In the next section we present numerical solution to the single-exciton problem. We find that the exciton binding energy E_b decreases as d increases and concurrently the momentum-space ground state wavefunction sharpens. Thus, the quantum size of an exciton $a_{ex}(d)$ increases with d. In Sec. III, we complement the single-exciton results with mean-field analysis of the uniform excitonic condensate ground state for varying carrier density n_{2D}. By comparing the exciton wavefunction obtained from the Wannier approximation with that in Sec. II, we obtain a quantitative criterion for the "diluteness" of an exciton gas. We conclude the paper with a remarks in Sec. IV.

II. SINGLE-EXCITON PROBLEM

Let us start with an electron and a hole in a double-layer system with $d = 0$. The eigenstates of this problem are obtained by solving the equivalent problem of a particle with mass m_r in a central attractive potential. Due to the rotational invariance in two dimensions[5] and the existence of the conserved Runge-Lenz vector,[6] the energy spectrum in the limit $d = 0$ is dependent only on the principle quantum number $n \geq 1$, $E_n = -4E_0/(2n-1)^2$ where $E_0 = e^2/\epsilon a_0$ is the energy scale associated with the problem. (Note that typical parameters $\epsilon \sim 10$ and $a_0 \sim 50$Å imply $E_0 \sim 30$ meV). The corresponding normalized ground-state wavefunction is given by $\psi_G(r) = \sqrt{8/(\pi a_{ex}^2)}\exp(-2r/a_{ex}) = \sqrt{2/(\pi a_0^2)}\exp(-r/a_0)$.[5] When $d \neq 0$, since the electron-hole interaction is given by $V_E(\mathbf{r}) = -e^2/\epsilon\sqrt{r^2+d^2}$, the differential equation for the radial component of the ex-

citonic wavefunction that cannot be analytically solved. Instead, we use the momentum-space Schrödinger equation

$$\frac{\hbar^2 k^2}{2m_r}\psi_\alpha(\mathbf{k}) + \int_{\mathbf{k}'} V_E(|\mathbf{k}-\mathbf{k}'|)\psi_\alpha(\mathbf{k}') = E_\alpha \psi_\alpha(\mathbf{k}) \quad (1)$$

where $\mathbf{k}$ is the two-dimensional wavevector, $\psi_\alpha(\mathbf{k})$ is the momentum-space eigenfunction with eigenvalue E_α, and $V_E(\mathbf{q}) = -V_A(\mathbf{q})e^{-qd}$ where $V_A(\mathbf{q}) = 2\pi e^2/\epsilon q$ is the Fourier transform of the intralayer Coulomb interaction in two dimensions. We focus on Eq.(1) projected onto the zero angular-momentum sector and obtain the eigenenergies and eigenfunctions by discretizing the integral equation and numerically diagonalizing the resulting matrix[7]

$$H_{mn} = \frac{u_n^2}{2}\delta_{mn} + \frac{u_n \Delta u}{2\pi}\tilde{V}(u_m, u_n) = \frac{u_m}{u_n}H^*_{nm}. \quad (2)$$

Here $\tilde{V}(u_m, u_n)$ is the angular-averaged dimensionless electron-hole interaction. Although the Hamiltonian (2) leads to bound and continuum states, since the excitonic internal states are only accessible at temperatures $T \geq E_0/k_B \sim 300$ K, in the following we only discuss the behavior of the ground state.

Figure 1 shows the numerically obtained ground-state energy of a single exciton as a function of interlayer distance d. At $d = 0$, the numerical result deviates from the well-known analytical answer by 10%; however, we have verified that this difference is solely due to discretization errors and can be systematically suppressed.[7] When $d/a_0 \ll 1$ first-order perturbation theory implies that the change in the ground-state energy is linear, $\delta E_G = E_G(d) - E_G(0) = 4E_0(d/a_0)$. At large d the excitonic binding energy is strongly suppressed; for example, when $d/a_0 = 10$ it is reduced to 10% of the binding energy at $d = 0$.

In Figure 2, we show the corresponding evolution of the ground-state wavefunction with increasing d. At $d = 0$ the normalized wavefunction is given by $\psi_G(k) = \sqrt{8\pi a_0^2}/(1+k^2a_0^2)^{3/2}$ and is reproduced by our numerical calculations. As d increases, we see that the momentum-space wavefunction sharpens and shows that the single exciton size $a_{ex}(d)$ increases with d.

These results show that a single exciton in a double-layer system is increasingly weakly bound, and becomes larger as the interlayer distance d increases. Therefore, although r_s is a good measure of the diluteness of electrons or holes, it is not a good measure of diluteness for the excitonic gas. To quantify this observation, in the next section, we study the evolution of a uniform excitonic condensate state as a function of $(d/a_0, r_s)$.

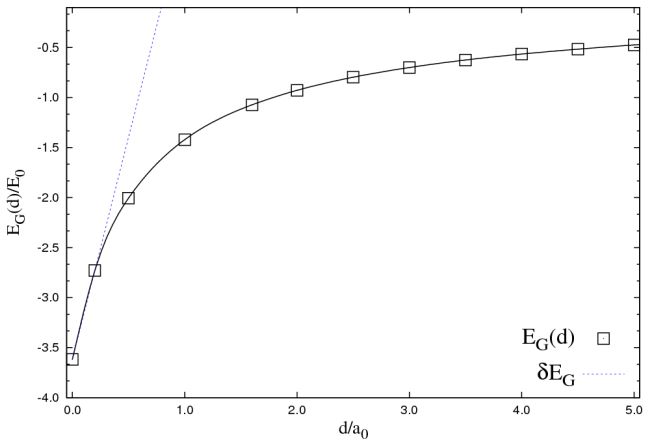

FIG. 1: (Color Online) Excitonic ground-state energy $E_G(d)$ as a function of interlayer distance d obtained from single-particle Schrödinger equation. The dotted line through $d = 0$ shows that at small d the change in the binding energy is linear, $\delta E_G = 4E_0(d/a_0)$, as expected from first-order perturbation theory. The binding energy is strongly suppressed at large d.

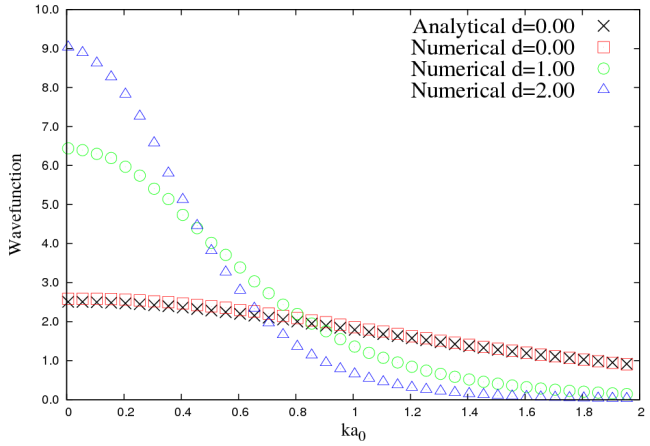

FIG. 2: (Color online) Ground state wave-function $\psi_G(k)$ for a single exciton as a function of interlayer distance d. The analytical (cross) and numerical (open square) solutions for $d = 0$ are consistent with each other. Their momentum-space width indicates that the exciton size is a_0. As d increases $\psi_G(k)$ sharpens and the size of the exciton, defined by the inverse-width of the momentum-space wavefunction, increases.

III. MEAN-FIELD ANALYSIS

To explore the uniform excitonic condensate state, we start with a double-layer system with electrons in the top layer and holes in the bottom layer that is separated by distance d. The Hamiltonian for such a system is a sum of the kinetic energy for electrons and holes, as well as the intralayer Coulomb repulsion $V_A(\mathbf{q})$ and the interlayer Coulomb attraction $V_E(\mathbf{q})$. We use the standard mean-field approximation[8,9,10] to obtain the mean-field Hamiltonian,

$$H = \sum_{\mathbf{k}} (e^\dagger_{\mathbf{k}}\, h_{-\mathbf{k}}) \begin{pmatrix} \xi_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta^*_{\mathbf{k}} & -\xi_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} e_{\mathbf{k}} \\ h^\dagger_{-\mathbf{k}} \end{pmatrix} \quad (3)$$

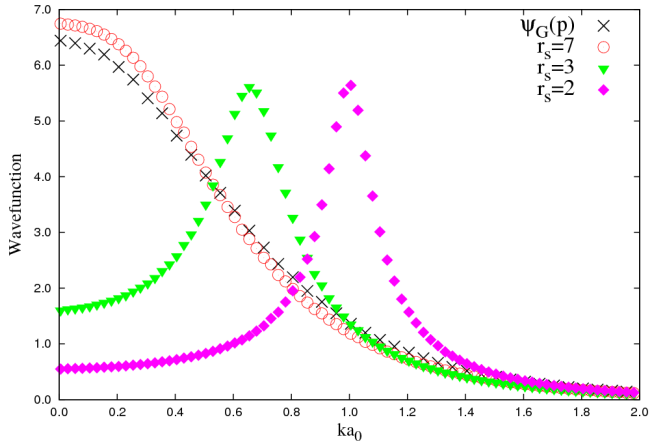

FIG. 3: (Color online) Comparison of the Wannier wavefunctions $\Phi(p) = \Delta_p/E_p$ obtained from the mean-field solutions for $r_s = 7$ (red circle), $r_s = 3$ (green triangle), and $r_s = 2$ (diamond), with the single-exciton wavefunction $\psi_G(p)$ (cross) for $d/a_0 = 1$. As r_s increases the Wannier wavefunction approaches the single-exciton result.

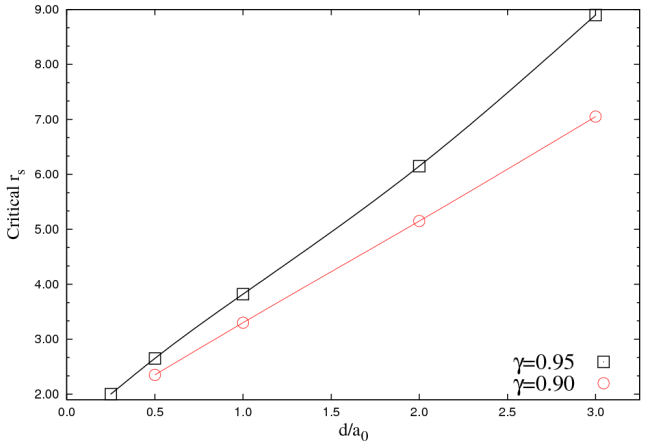

FIG. 4: (Color online) Interlayer-distance dependence of the critical r_s value obtained using the constraints $\gamma = 0.90$ (bottom) and $\gamma = 0.95$ (top). $r_{sc}(d)$ provides a quantitative way to characterize the diluteness of an excitonic gas by comparing the Wannier wavefunction $\Phi(k)$ with the single-exciton solution $\phi_G(k)$.

where $e^\dagger_{\mathbf{k}}$ ($h^\dagger_{\mathbf{k}}$) is the creation operator for an electron (hole) with two-dimensional momentum $\hbar\mathbf{k}$ in the top (bottom) layer, $\xi_{\mathbf{k}}$ is renormalized electron (hole) dispersion that takes into account the interlayer capacitance and intralayer exchange energy, and $\Delta_{\mathbf{k}}$ is the excitonic order parameter associated with the coherence between the electron and the hole bands in the two layers. We consider an isotropic excitonic-condensate order parameter and obtain the following self-consistent mean-field equations[9,10]

$$\xi_k = \varepsilon_k + V_C - \mu - \int_{\mathbf{k}'} V_A(|\mathbf{k}-\mathbf{k}'|)\langle e^\dagger_{\mathbf{k}'} e_{\mathbf{k}'}\rangle \quad (4)$$

$$\Delta_k = \int_{\mathbf{k}'} V_E(|\mathbf{k}-\mathbf{k}'|)\langle h_{-\mathbf{k}'} e_{\mathbf{k}}\rangle \quad (5)$$

$$n_{2D} = \int_{\mathbf{k}} \langle e^\dagger_{\mathbf{k}} e_{\mathbf{k}}\rangle = \frac{1}{2}\int_{\mathbf{k}} \left(1 - \frac{\xi_k}{E_k}\right) \quad (6)$$

where $\varepsilon_{\mathbf{k}} = \hbar^2k^2/2m_e = \hbar^2k^2/2m_h$ denotes the electron (hole) band dispersion, $V_C = 2\pi e^2 n_{2D}/\epsilon$ is the capacitive energy cost, and μ is the (electron and hole) chemical potential determined implicitly by Eq.(6). The self-consistent excitonic order parameter is determined by $\langle h_{-\mathbf{k}} e_{\mathbf{k}}\rangle = \Delta_k/2E_k$, and $\pm E_{\mathbf{k}} = \pm\sqrt{\xi^2_{\mathbf{k}} + \Delta^2_{\mathbf{k}}}$ denote dispersion of the quasiparticle bands that result from Hamiltonian (3). We solve Eqs.(4)-(6) iteratively for a given $(d/a_0, r_s)$ to obtain the self-consistent order parameter Δ_k and quasiparticle energy dispersion E_k. To explore the dilute exciton limit, we recast Eq.(5) in terms of $\Phi(p) = \Delta_p/E_p$, and note that for $\Delta_p \ll \xi_p$ Eq.(5) reduces to the single-exciton Schrödinger equation in momentum space, Eq.(1). This permits a quantitative comparison between the ground-state exciton wavefunction $\psi_G(p)$ and the Wannier-exciton wavefunction $\Phi(p)$.

Figure 3 compares the Wannier wavefunction $\Phi(p)$ at $d/a_0 = 1$ for different values of r_s with the single-exciton wavefunction $\psi_G(p)$. We see that r_s increases the Wannier wavefunction approaches the single-particle result, as expected. Note that for small r_s, the Wannier exciton wavefunction $\Phi(p)$ is peaked at finite momentum because the excitonic order parameter Δ_p is maximum and ξ_p is minimum at the Fermi momentum. However, as r_s increases, for any given d, the peak in Δ_p shifts towards the origin and so does the maximum of the Wannier wavefunction.

To quantify the proximity between the Wannier and the single-exciton approach, we consider the overlap $\gamma(d/a_0, r_s)$ between the two (real) wavefunctions

$$\gamma(d/a_0, r_s) = \int \frac{d\mathbf{k}}{(2\pi)^2}\Phi^*(k)\psi_G(k). \quad (7)$$

A high overlap value $\gamma(d/a_0, r_{sc}) \sim 1$, allows us to define a critical value of $r_{sc}(d/a_0)$ such that for $r_s \geq r_{sc}$ the single-exciton result provides an excellent substitute for the mean-field analysis. Figure 4 shows the critical $r_{sc}(d)$ obtained using $\gamma = 0.90$ and $\gamma = 0.95$. We see that for typical values of d the critical r_{sc} scales linearly with d/a_0. It implies, for example, that approaching the dilute-limit at $d/a_0 = 3$ will require reducing the carrier density by a factor of 5 from the corresponding value for the dilute limit at $d/a_0 = 1$.

IV. DISCUSSION

The subject of excitonic condensation in double-layer systems has been extensively explored in the literature; the properties of a single exciton in a double-layer system, however, have not been. In this paper, we have

obtained the ground-state wavefunction and the ground-state energy for a single exciton as a function of interlayer distance d. By comparing our results with those from a mean-field analysis of the uniform excitonic condensate, we have obtained the critical value $r_{sc}(d)$ that is used to determine when the exciton gas for a given interlayer distance d is "dilute".

Our analysis provides a quantitative picture of a single exciton in double-layer system with $d \neq 0$ where analytical solution for the excitonic wave-functions is not possible. It shows that as d increases, due to the weakened electron-hole Coulomb interaction, the exciton size $a_{ex}(d)$ increases.

We note that the Wannier approximation for excitonic wavefunction is based on a mean-field analysis that usually over-estimates[8] the excitonic order parameter Δ_k. In particular, in double layer systems, it is known that the uniform condensate becomes unstable[11] when d is larger than a critical layer separation d_c. Thus, when fluctuations around the mean-field state are taken into account, the critical value of r_s for a given $d \sim d_c$ will change substantially. Our mean-field analysis is based on a uniform excitonic condensate state. Due to dipolar repulsion between excitons, the uniform state is unstable towards formation of a crystalline excitonic condensate[12] in the region $\sqrt{r_s} \ll d/a_0 \ll r_s$. Since our calculations lie outside this parameter range, we have focused only on the uniform state; the question of a "dilute" exciton limit in a crystalline excitonic condensate, however, remains open.

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[1] See *Bose-Einstein Condensation*, edited by A. Griffin, D.W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, 1995) and references therein.

[2] S.A. Moskalenko and D.W. Snoke, *Bose-Einstein Condensation of Excitons and Biexcitons* (Cambridge University Press, New York, 2000).

[3] J.M. Blatt, K.W. Böer, and W. Brandt, Phys. Rev. **126**, 1691 (1962).

[4] See "Macroscopic coherent states of excitons in semiconductors" by L.V. Keldysh, in[1].

[5] X.L. Yang, S.H. Guo, and F.T. Chan, Phys. Rev. A **43**, 1186 (1991).

[6] W. Dittrich, Am. J. Phys. **67**, 768 (1999).

[7] W.A. Karr, C.R. Jamell, and Y.N. Joglekar, arXiv:0910.0574.

[8] J.W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison Wesley, Massachusetts, 1988).

[9] P.B. Littlewood and X. Zhu, Phy. Scrip. **T68**, 56 (1996).

[10] C.H. Zhang and Y.N. Joglekar, Phys. Rev. B **77**, 233405 (2008).

[11] S.De Palo, F. Rapisarda, and G. Senatore, Phys. Rev. Lett. **88**, 206401 (2002).

[12] Y.N. Joglekar, A.V. Balatsky, and S. Das Sarma, Phys. Rev. B **74**, 233302 (2006).